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# Program Managers Questions for LL13-MatModelRadDetect-2Jf

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## Disclaimer



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# Program Managers Questions for LL13-MatModelRadDetect-2Jf

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***Specific Program Management Questions***

Answers are provided in blue.

**Scientific/Technical Soundness:**

1. What are the current project goals and are they well defined?

The major project goals are three-fold:

1) to determine the mechanisms of polarization of TlBr detectors related to electrical contact materials, and enable the rational design of optimal contact stacks for maximum detector longevity;

2) to elucidate the carrier trapping propensity of dislocations in CdTe/CZT and determine whether this depends on type and decoration of the dislocations; evaluate whether dislocation engineering (out of scope of this project) can optimize CZT detector performance;

3) to discover if (and how) a glass material can make a high-performance host for a scintillator, by understanding how atomic structure differences associated with composition and forming conditions affect carrier transport.

2. Is the technical program plan reasonable and likely to achieve the project objectives?

A systematic plan is in place to make progress against the objectives and to maximize the likelihood of success. Milestones define key activities along the way to deliverables. Specific milestones and deliverables are outlined in the answer to question 6 in the "Management/Execution" section below. The general program plan consists of ground-laying work in the first one-to-two years, followed by more discovery-type activities in the third year toward the ultimate goals of materials design. Along the way, enabling knowledge will be generated that will be helpful for broad materials optimization efforts in the three technology areas that comprise the focus of this project. The main outcomes of this project are expected to be answers to "how" and "if"-type questions (*e.g.,* "can a glass perform nearly as well as a crystalline material for scintillators?", "how can electrical contacts make TlBr detectors survive longer? what properties of the contacts are needed?", etc.). The answers will be valuable, even if the follow-on materials design/discovery goals are only partially achieved.

More specifically, for the TlBr contacts work, a progression of study is planned, beginning with understanding the role of different metal impurities in creating deep traps in TlBr, followed by study of Fermi-level pinning of different metals, then determination of different compounds that may exist (or

be inserted) between TlBr and metal, along with computation of those compounds' relevant properties (*e.g.*, deep traps, band offsets, diffusive permeability). By comparing with experimental results, this progression of calculations will enable the mechanisms responsible for detector degradation (and longevity) to be established. Then, by identifying the required set of target properties to maximize longevity, given those mechanisms, design of optimal contact stacks can proceed rationally.

For the glass scintillator work, the first year is focused on establishing and validating methods to control the generation of glass models that can be related to experimental conditions and to analyze the correlation between atomic and electronic structure. Validation of the methods will use well-studied glasses with available experimental data. From that groundwork, the project will proceed to apply the methodologies to explore a wider variety of glass chemistries, with the goal of discovering a "structural vector" that improves electronic transport in glasses. Finally, the task evolves to searching for ways to design a glass with the desired structural characteristics; ideally, this latter task would involve both computational and experimental efforts to generate ideas on how to satisfy the design principles established from the earlier work.

The work on CdTe dislocations is more straightforward and follows a simple progression of increased complexity toward more realistic structures. As the complexity increases, the limiting factor of the scope of work is the increased computational cost of generating and analyzing the atomistic models. This risk is mitigated by access to scalable codes and large supercomputers (see the answer to question 4 below). In the end, the number of different structures that can be studied will be modest for those requiring very large numbers of atoms (dilute impurities and kinks).

3. Please describe technical progress to date and indicate how well it meets the agreed to milestone and deliverable schedules.

The two scheduled deliverables to-date, plus the annual report to stakeholders, have been completed and submitted.

Major technical achievements include:

**For TlBr:** (i) The electronic properties of a dozen metal impurities have been determined, and ranked lists of expected top-performing anode and cathode metals were generated from the data, from the point of view of metal-induced deep traps in the semiconductor. (ii) The band alignment of $TlBr_{1-x}Cl_x$ with TlBr was determined, across the whole composition range of Cl. TlBrCl is a compound that can be formed between the metal and TlBr by treating the surface with HCl and represents a simple engineered material in the contact stack with available associated experimental data. The electronic properties and diffusion rates of of metal impurities in TlBrCl were computed to learn how the HCl treatment may improve longevity (see the answers to questions 5 and 6 below for further details). We also computed the absolute work functions of the compounds to understand band bending and Schottky barriers at the contacts. (iii) We have begun to compute the thermodynamic

stability of various compounds that may form at the interface between the metal and TlBr or TlCl, and to compute their electronic properties. We completed the thermodynamic analysis for $Tl_2PtCl_6$, which is stable for Cl-rich conditions and thus may serve as a sink for Pt impurities. (See the answer to question 6 below for further details.) Next steps are to compute the electronic properties of the compound.

**For glass scintillators:** We validated our glass model generation procedure and the potentials used for same, for silica and sodium silicate glasses. We evaluated the range of computational control over structure variability by tuning simulations parameters that are analogous to experimental variables. We developed a novel analysis method to correlate local structural motifs with electronic structure properties, particularly trapping propensity of band-tail states. We applied these methods to compare the atomic structures and electronic properties of silica and several compositions of sodium silicate glasses. A deliverable report detailing these results was completed. One major finding was a detailed explanation of how the disorder-inducing sodium atoms in sodium silicate create significantly worse charge transport than in pure silica, an effect which scales with sodium content.

**For CdTe/CZT dislocations:** We generated and relaxed accurate structural models of a variety of straight [-110] dislocations in CdTe: 1 screw dislocation, 3 Cd-core edge dislocations with different core structures, and 3 Te-core edge dislocations with analogous core structures. The relative thermodynamic stability of each core structure was determined. The electronic density of states as a function of radial distance from the dislocation cores were computed and analyzed. We found a number of interesting features, including deep and shallow traps associated with different dislocation core structures. Certain dislocations exhibit hole or electron traps that are delocalized along the dislocation line, *i.e.*, they provide efficient conduction of trapped carriers along the dislocation. This latter result suggests the possibility of enhancing 1D conduction in crystals, if certain dislocations could be favored and aligned. A short conference paper outlining the results was delivered, and a more detailed manuscript is in preparation, to meet a scheduled deliverable. A slight staffing shortfall mid-year resulted in the delay of the fully detailed manuscript, but presently we are fully staffed.

4. What additional unresolved technical issues can you anticipate that may potentially cause difficulties?

A risk factor for the CdTe dislocation work in the second and third years is the large size of the simulation cells required. The straight dislocation models need about 600-700 atoms and are only 1 unit cell thick (with periodicity) in the line direction. To model a kinked dislocation or a dislocation with a realistically low concentration of impurities (as opposed to an effective “wire” of impurities alongside the dislocation line), a thicker supercell is needed to explicitly treat a longer segment of the dislocation. For example, if 4 unit cells of length need to be treated explicitly, then a system size around 2500 atoms is required. This is approaching the limit of standard DFT codes (although still

doable with effort and long computer time), but is well within the limits of the semi-empirical methods we use to setup the initial structure. We can mitigate the computational difficulty of the final DFT step on these large systems by using scalable in-house DFT codes at LLNL on our largest supercomputer (*i.e.,* qb@ll and MGmol on the vulcan/sequoia BG/Q system). For example, the qb@ll code has recently been demonstrated to scale nearly linearly to over 65,000 cores on vulcan for a system with 2000 atoms. This allows us to perform DFT relaxations on very large systems in reasonable wall-clock time by trading off computational cost. We have access to the vulcan supercomputer at no direct cost to NA-22.

For the glass scintillator work, technical issues are not anticipated, but a possible result is that we discover little freedom to design a glass with drastically improved carrier transport (preferably more than an order of magnitude improvement). However, as a high-impact, high-risk portion of the project, this possibility is acceptable. Current indications are that optimal glasses have not been discovered yet, and that results to-date are far from the theoretical maximum, so we are hopeful that at least some improvement can be designed in. One avenue with great potential is to attempt the analog of what has enabled high-performance organic crystal and plastic scintillators, namely to create a mixture with percolated conducting “trap” impurities (in this case, the “impurities” could be either dopants or more likely a secondary glass phase). Part of the team for this project contributed to the discovery of that basic science knowledge, which enabled high-performance organic and plastic scintillators to be developed for a different project.

5. Has there been any progress in resolving the mechanism of contact lifetime improvement in chlorinated TlBr contacts? Is the observed experimental effect large?

The mechanism of detector longevity improvement with contacts formed on chlorinated TlBr is currently being resolved and is a main thrust of active work. Some of the effects are understood, but other mechanisms that possibly contribute are mostly hypotheses, which we are trying to prove by working both theory and experiment (with our DNDO collaborators). One thing we have determined is that hole blocking from the contacts plays a role. Our calculations, combined with experiments, have allowed us to map with good accuracy (~0.05 eV) the absolute band edges of TlBrCl across the entire Cl composition range (including TlBr, of course). The results show that there is a significant valence band offset that blocks hole injection from the metal into the semiconductor, but for most Cl contents the conduction band offset is either small or slightly negative (non-blocking for electron injection from the contacts). The end result is that signal current (predominantly electron current) is not hindered from exiting the crystal when excited by a gamma ray, but the blocked hole injection reduces the electronic current transients and background. A manifestation of this phenomenon is that field annealing is not required for the chlorinated devices. The precise mechanism that relates this to improved longevity is still being studied. Some possible effects include:

reduced vacancy/impurity migration rate through the Cl-rich material, a shift in impurity metal deep levels in the Cl-rich material, a shift of the electrochemical potential at the interface (modified Fermi-level pinning), or locking of the metal impurities in a stable compound at the interface. The first three hypotheses have not yet been proven/supported by first principles calculations, but are being actively investigated. The fourth effect has recently been shown to be at least plausible: with typical Pt contacts, a $Tl_2PtCl_6$ compound was found to be thermodynamically stable for Cl-rich conditions (see additional details in the answer to the following question), while such a compound is not stable for TlBr. Additional resolution of the responsible mechanisms for longevity improvement is a high priority effort currently, since it can strongly direct how we might design an optimal material stack by identifying the critical material parameters.

The observed experimental effect is significant. Some HCl treated devices have been demonstrated to remain stable for about 1 month, but the effect does depend on choice of contact metal and processing, and is still not fully understood.

6. Of the Tl-Br-M and Tl-Cl-M compounds that form ternaries, have any been tested experimentally to see if they block polarization?

We are just beginning to work on these compounds and are devising an experimental plan with A. Conway *et al.* at LLNL. The first compound we began investigating may form between TlCl and Pt, which corresponds to a possible interphase compound formed in typical devices made by that team. Recent, relatively high-performing devices have chlorinated surfaces from HCl treatment on which Pt metal contacts are deposited. Theory suggests that under Cl-rich conditions a $Tl_2PtCl_6$ compound is stable, while the Br analog is never more stable than TlBr+Pt. This is a possible advantage to having the TlBrCl layer, in that formation of the $Tl_2PtCl_6$ compound may stabilize and “freeze-in” Pt impurities, which otherwise could make their way into the TlBr and act as deep carrier traps. This is a possible mechanism to avoiding polarization. Our collaborators have new device samples with Pt contacts that separated from the semiconductor. This device presents an opportunity to experimentally study the chemistry at the interface between the Pt and chlorinated TlBr and look for the $Tl_2PtCl_6$ compound. Those experiments are currently underway.

7. For the glass host calculations, how did you determine how many atoms must be considered in this disordered material to obtain accurate electronic properties and melting behavior? How much computational effort did this entail?

We test bigger systems using the empirical potentials to check that the atomic structure does not change (to verify that finite size effects from periodic boundary conditions do not affect the local structure). For example, we tested sodium silicate systems with ~700, 1500, and 2500 atoms to determine that the melt-quench structure was converged for the 700 atom system, at least

for local structure. When we choose the system size, we compromise slightly on the mid-range structural order in favor of smaller systems that still correctly describe the localized structures. The localized structures are responsible for trapping/carrier transport much more than mid- or long-range order.

We perform structure comparisons using our suite of structure characterization tools, including atom correlation functions, $Q^n$ numbers, angular distributions, ring distributions, etc. We seek to keep system size relatively small (< 1000 atoms, if possible), so that we can run the entire system with DFT in a reasonable time (on the order of a week, or up to a month) to extract the electronic properties. Use of an ensemble of structures, as long as the periodic boundary conditions are not affecting the local structure, allows us to sample effectively larger volumes without needing a larger system size by using time averages instead of spatial averages. The ergodicity principle guarantees that these averages are equivalent.

The computational effort to perform the semi-empirical melt-quench simulations for system sizes of thousands of atoms is not very large (on the order of days), with some overhead associated with performing the structural characterization analyses. However, the ultimate DFT cost to subsequently extract the electronic properties nominally scales as the number of atoms cubed (or in practice to a power of about 2.5), driving the desire for reasonably small systems size. The DFT cost for systems with thousands of atoms is large enough that we only perform selected convergence tests of the electronic density of states, to ensure it is the same for larger and smaller system sizes.

**Management/Execution**

1. Who are the primary individuals working on this project and what are their roles? Please provide the background of these individuals relevant to their roles. Are there key individuals outside your organization, students or subcontractors that assist your project?

The key individuals, their backgrounds, and roles on this project are:

**Vincenzo Lordi** is the principle investigator for the project, responsible for project management and direction, oversight, and application of the theoretical methods. He has 15 years experience in materials modeling, spanning from quantum-mechanics-based first-principles methods to semi-empirical potential methods to meso-scale coarse-grained methods to continuum-level device modeling. His expertise ranges across density functional theory, quantum Monte Carlo, kinetic Monte Carlo, molecular dynamics, and TCAD device modeling. He also has extensive experience in experimental crystal growth; material characterization using optical, X-ray and electron spectroscopy as well as electron microscopy; and device fabrication. Much recent work has focused on studying the effects of defects in semiconductors on their electronic and optoelectronic properties, including more than 6 years as PI of NA22-funded projects studying materials for room-

temperature radiation detectors. A characteristic of his work is the close coupling of theory with experiment. B.S.E in chemical engineering from Princeton, M.S. in electrical engineering from Stanford, Ph.D. in materials science & engineering for Stanford, Hertz Fellow, Lawrence Fellow. He led industrial R&D for a new product at KLA-Tencor Corp. before joining LLNL.

**Daniel Åberg** is a staff member in the Materials Science Division of LLNL. He is an expert in first-principles materials modeling, including density functional theory and beyond-DFT methods such as hybrid functionals and the *GW* method. He has been a core member of the radiation detector materials modeling team at LLNL since beginning as a post-doc in 2006, and has focused on CdTe and CZT in recent years. He also has experience in modeling the electronic structure of silica glass and leads a computational effort studying the physics of crystalline scintillators. His primary role will be to support the postdoc working on dislocations in CdTe. He will play a consulting role on the glass scintillator task as well.

**Nicole Adelstein** is a postdoctoral fellow in the Quantum Simulations Group of the Materials Science Division of LLNL. She hold a Ph.D. in materials science from the University of California at Berkeley, where she studied electronic, ionic, and polaronic transport in rare-earth phosphates using first-principles methods. Her recent work at LLNL has included studying the electronic and magnetic properties of surface defects in quartz and silica, as well as the structure of glassy materials. Here role is on the glass scintillator aspect of this project, generating atomic structures and analyzing their electronic properties.

**Joel Varley** is a postdoctoral researcher in the Materials Science Division at Lawrence Livermore National Laboratory. He received his PhD in 2011 from the Department of Physics at the University of California, Santa Barbara and was a postdoctoral researcher in the Department of Chemical Engineering at Stanford University from 2011 to 2013. His research interests include first-principles calculations of materials with an emphasis on understanding and engineering the effects of doping and defects in semiconductors for electronic and (photo-)catalytic applications. His role is to support the TlBr tasks of this project, by performing point defect and band offset calculations.

**Keith Ray** is a postdoctoral fellow in the Quantum Simulations Group of the Materials Science Division of LLNL. He studied the binding and transport of gas molecules in nanoporous metal organic frameworks using van der Waals corrected density functional theory for his Ph.D. research in physics from the University of California at Berkeley. His current work at LLNL consists of studying defect formation and migration in semiconductors, noise sources in qubits, hydrogen storage in nano particles, and ionic conduction in solid electrolyte materials. His primary role is to study interphase compound formation in TlBr contacts and their properties relevant to polarization.

**Kyoung Kweon** is currently a postdoc of Chemical Engineering at the University of Texas at Austin, where she also completed her Ph.D. in Electrical & Computer Engineering. Her recent research was focused on developing a better understanding of oxide materials for energy applications using first principles quantum mechanical calculations. In particular, her primary efforts were devoted to examining the structural and electronic properties of metal oxides, along with molecular mechanisms underlying the catalytic reactions on their surfaces, such as water splitting and oxygen reduction/evolution reactions. Her Ph.D. work was focused on studying the structural and electronic properties of group IV semiconductors and amorphous silica, particularly the effects of defects and impurities. She has extensive experience in a wide variety of electronic structure techniques for computational materials science. Kyoung will join LLNL as a postdoc in the Materials Science Division in January or February 2015. Her primary role will be on CdTe dislocation tasks, but she will also contribute to the TlBr and possibly the glass scintillator tasks.

**Vasily Bulatov** is a leading expert in dislocation theory and mesoscale materials modeling, and original co-author of the ParaDIS dislocation dynamics code. He has authored or co-authored numerous papers and books/book chapters on dislocation structure and dynamics. Currently chief scientist in the Materials Science Division at LLNL, former Teller Fellow, William and Mary Greve Foundation Fellow, and Fellow of the American Physical Society. He will serve in a consulting role, contributing expertise for the dislocation portion of the project.

In addition, we have worked with three summer students as part of the LLNL Computational Chemistry & Materials Science summer institute, who have contributed to work on CdTe dislocations (Eunae Cho, currently at Samsung Research, Korea; and Michael Skarlinski, University of Rochester) and glass scintillator structure generation (Christopher Olson, North Dakota State University). They all had experience in first-principles materials modeling. Also, for the TlBr work, we collaborate closely with Adam Conway *et al.* at LLNL and Kanai Shah *et al.* at RMD, Inc., who are funded through DNDO for complementary experimental studies on that material. Conway's work is particularly focused on experimental studies of the contact interfaces. These experimental teams have expertise in crystal growth, device fabrication, electrical testing, device physics, and materials characterization.

2. Is this project team engaged in similar work sponsored by DNDO, DTRA, DOE-NE or other NNSA offices? If so, please describe technical area and application area.

No, but for the TlBr tasks, we are collaborating with experimental partners who are funded by DNDO (Conway, *et al.* at LLNL and RMD, Inc.).

3. Is this project team engaged in similar work sponsored by other WFO or IWFO? If so, please describe how the technical work is complementary and integrates into this NA-22 sponsored effort.

Generally, no. However, the PI and some project members are engaged in complementary work in different fields using similar methods. For example, Lordi and Varley use hybrid density functional theory to analyze the electronic properties of defects and interfaces in semiconductor materials for thin-film solar cells, for a project sponsored by DOE/EERE. Adelstein is involved in a project sponsored by DOE/EERE on using density functional theory to explore atomic transport through solid electrolytes for rechargeable batteries.

4. Do you have any publications or presentations that you have prepared from this effort? Please be sure to upload and properly account for all reports or publications generated by this project into webPMIS?

All reported publications have been uploaded to webPMIS. Several conference presentations (oral and poster) have been given. One manuscript has been submitted. One report has been submitted to NA-22 as a deliverable. All quarterly reports are up to date in webPMIS. An invited presentation at the 2013 NSS/RTSD in Seoul had to be withdrawn due to travel restrictions. Two additional manuscripts are currently in preparation.

5. Who are competitors for developments of this or similar work in the labs, universities, and industry and how are you distinguishing yourselves from them?

While a number of researchers are engaged in generally similar work of using first principles calculations to study defects in materials, the application of these techniques in the application spaces of this project is mostly unique to this work.

Our work on TlBr currently has few direct competitors, particularly with the focus on electrical contact interfaces. Theoretical work on TlBr defects in general continues to be or has recently been pursued by groups at MIT (Tuller), Berkeley (Chrzan/Haller), and ORNL (Singh), but have all focused on point defects. Our work is further distinguished by tight collaboration with experimental teams (at LLNL and RMD), who are working in coordination with us to understand and improve the detector performance through contact stack design and optimization.

Our glass scintillator work is unique and has invented a new unique analysis of glass electronic structure correlated with atomic structure, although the analysis has been partly inspired by others' work in the literature. The generation of glass structure models is an old field, but one that is still vibrant, as understanding disordered systems continues to be a hot challenge in materials science. The connection to electronic structure is less explored, since usually glasses are not considered as conducting electronic materials. Some recent work in the literature [S. Ispas, M. Benoit, P. Jund, & R. Jullien, PRB (2001)] has explored the localization of states in sodium silicate glass (with less sodium than we considered), but has not analyzed the atomic/electronic structure correlation in the detail we have. In addition, much of the work was done long enough ago that computing power did not allow the treatment of a significant ensemble of structures or of larger system sizes,

as we are able to do. For example, we are able to better sample the statistical structural variations (atomic and electronic) by using ensembles of 30-50 structures of ~700 atoms each, whereas the prior work used 2 snapshots of 90 atoms each.

For the CdTe dislocation work, there is some competition from a group at the University of Toledo led by Prof. Yanfa Yan that has been doing similar investigations in the context of CdTe solar cells. Prof. Yan, *et al.* have used aberration-corrected electron microscopy to image some dislocation core structures, which they fed into density functional theory calculations to obtain the electronic structure. Their work has proceeded mostly concurrently with ours, but utilized much smaller and periodic supercells in the calculations. The use of the small, periodic supercells led to spurious interactions in their results and non-physical dispersive defect states from the dislocation cores. That group has since discovered our result that much larger supercells, preferably with open boundary conditions, are required to obtain results consistent with experiment. (That group has spoken about their puzzling simulation results that did not agree with micro-cathodoluminescence experiments, which they ultimately explained were the result of the overly constrained supercells.)

6. Please delineate planned project milestones and deliverables.

The main deliverables consist of publications and reports to collaborators and stakeholders. Various milestones track major activities toward project deliverables. Summary tables of all milestones and deliverables are copied below, colored and sorted chronologically by task. Deliverables are highlighted in bold.

**SUMMARY TABLE OF MILESTONES AND DELIVERABLES FOR FY2014**

| Due Date | M/D | Task # | Description |
|---|---|---|---|
| 09/30/2014 | M | 1 | Complete construction of atomistic interface model for 1 relevant metal |
| 11/30/2013 | M | 2 | Validate structure and electronic density of states of amorphous silica test-case |
| 02/15/2014 | M | 2 | Construction of first complete glass model |
| 03/30/2014 | M | 2 | Analysis of structure factor of model and comparison to experimental data from literature |
| 08/30/2014 | M | 2 | Completion of two comparative glass models |
| **09/30/2014** | **D** | **2** | **Deliver report contrasting atomic structure motifs of two glass models and validation data to NA-22** |
| 01/31/2014 | M | 3 | Obtain electronic gap states of a single straight edge dislocation, as a function of distance from the core |

| | | | |
|---|---|---|---|
| 03/30/2014 | M | 3 | Use empirical potentials combined with density functional theory to generate structures and determine the electronic states of a set of at least 6 dislocations in CdTe |
| **06/30/2014** | **D** | **3** | **Submit manuscript on atomic and electronic structure of straight dislocations in CdTe to a peer-reviewed journal** |

**SUMMARY TABLE OF MILESTONES AND DELIVERABLES FOR FY2015**

| Due Date | M/D | Task # | Description |
|---|---|---|---|
| 02/28/2015 | M | 1 | Complete construction of atomistic interface model for at least 2 relevant metals |
| 04/30/2015 | M | 1 | Analysis of interface chemical thermodynamics, in terms of stable interface phases |
| **09/30/2015** | **D** | **1** | **Deliver report on chemical thermodynamics of TlBr–metal interfaces (at least 2 relevant metals) to NA-22** |
| 02/15/2015 | M | 4 | Construct interface models with heterostructure material between TlBr and metal |
| 07/15/2015 | M | 4 | Determine electronic states and Fermi-level pinning of interfaces |
| **09/30/2015** | **D** | **4** | **Deliver report on heterostructure effects on device stability of TlBr detectors to NA-22** |
| **09/30/2015** | **D** | **5** | **Submit manuscript on electronic structure of two glass hosts to peer-reviewed journal** |
| 01/30/2015 | M | 6 | Use empirical bond-order potential to generate initial structure of a kinked screw |
| 03/30/2015 | M | 6 | Relax structure of kinked screw dislocation with density functional theory |
| 07/15/2015 | M | 6 | Evaluate electronic density of states for kinked screw dislocation |
| **09/30/2015** | **D** | **6** | **Submit manuscript on atomic and electronic structure of a kinked dislocation in CdTe to a peer-reviewed journal** |

**SUMMARY TABLE OF MILESTONES AND DELIVERABLES FOR FY2016**

| Due Date | M/D | Task # | Description |
|---|---|---|---|
| 03/30/2016 | M | 7 | Evaluate electrochemical potentials at interfaces from metal work functions |
| **05/30/2016** | **D** | **7** | **Deliver candidates for optimal TlBr contact structure/process to RMD and LLNL collaborators** |

| | | | |
|---|---|---|---|
| **09/30/2016** | **D** | **7** | **Submit manuscript on improved contact design for TlBr detectors to peer-reviewed journal** |
| 01/30/2016 | M | 8 | Compare effects of composition on atomic and electronic structure of glasses |
| 03/01/2016 | M | 8 | Establish experimental collaboration to test predictions |
| 06/30/2016 | M | 8 | Determine electronic transport coefficients for modeled glass structures |
| **07/15/2016** | **D** | **8** | **Suggest steps for optimizing scintillator glass to experimental collaborators** |
| **09/30/2016** | **D** | **8** | **Deliver report on chemical/process/composition trends of glass hosts for scintillators to NA-22** |
| 03/30/2016 | M | 9 | Evaluate electronic properties of key impurities in straight dislocation core |
| 07/15/2016 | M | 9 | Use experimental data along with simulations to evaluate contributions of bare and decorated dislocations on carrier transport in CdTe |
| **09/30/2016** | **D** | **9** | **Submit manuscript on electronic properties of dislocation networks in CdTe to peer-reviewed journal** |

7. Do you anticipate any additional changes?

The current project milestones and deliverables were revised from an originally-proposed set, based on revisions to the funding allocation. Additional changes are not anticipated.

8. Is the technical program plan reasonable and likely to achieve the project objectives by the end of the project?

Please see the answer to question 2 in “Scientific/Technical Soundness” above.

9. Why is your spending rate so low? You spent only $252,000 and carried over $1M dollars in FY14 and have spent $0 so far in FY15.

This project was originally selected for a FY13 start, but funds were not received until Sept 2013 and at a reduced level. (Original project budget was $660/680/700K; allocated funds were $300/500/500K.) When funds were allocated in Sept 2013, a revised LCP was submitted and approved, which essentially shifted work to FY14/FY15/FY16 at the revised funding levels. Subsequent years’ funding were allocated, respectively, at the beginning of FY14 and FY15, but were carried over for spending as outlined in the revised LCP. The $253K spending in FY14 actually corresponds to a carryover of $47K against the first year plan of $300K. That $47K carryover resulted from a 2-month delay in the hire of postdoc Keith Ray. The $500K received in Nov

2013 is intended for FY14 spending and was carried over. The third year funding of $500K was recently allocated ($98K received) in late Oct 2014. Thus, there appears to be a carryover of over $1M, but this is simply due to the timing of funds received and the shifted project schedule. Spending in FY15 as of 10/25/2014 was $24K. Accounting delays have presumably caused those charged not to appear yet. The spend rate is on target, with spending scheduled to increase when the new postdoc begins in January 2015 (question 11 below).

10. You are missing the FY14 final report and two other deliverables. Please turn them in and update your publications.

These have been entered into webPMIS. The final report was submitted late due to confusion over it being required for this project.

11. Is your postdoc fully on board to start the CdTe/CZT task?

A new postdoc has been hired for this task: Kyoung Kweon from the Univ. of Texas at Austin. She will begin in FY15 Q2 (January 2015 target start date).

**Potential User Impact**

1. What end user agencies with non-proliferation, counter-proliferation, or counter-terrorism applications might be expected to be interested in the capabilities of the technology being developed in this effort? What contacts, if any, have been made with these organizations and have they shown an interest or made suggestions?

Since the main outcome of this work is essentially improvement in the cost-to-performance ratio of some leading candidate materials for high-resolution room-temperature gamma detectors through the use of rational theory-based design, the end user agencies in need of these improved detectors for their non-proliferation or counter-proliferation missions are expected to be interested. Such agencies include DHS/DNDO, DoD/DTRA, as well as NNSA. Direct contact with these organizations has not been made, since the pipeline for the outputs of this project to provide them with improved detectors is through the detector developers. However, we remain engaged with these end user agencies, for example, through our collaboration with the DNDO-funded TlBr team. DNDO has expressed interest in our work in this area and has invited us to participate and present at a past program review meeting.

Our work in general is expected to impact the development and availability of improved materials for future higher performance, lower cost detectors, which the end user agencies can then leverage.